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Supporting information for article:

Compressibility of structural modulation waves in the chain compounds BaCoX2O7 (X = As, P); a powder study

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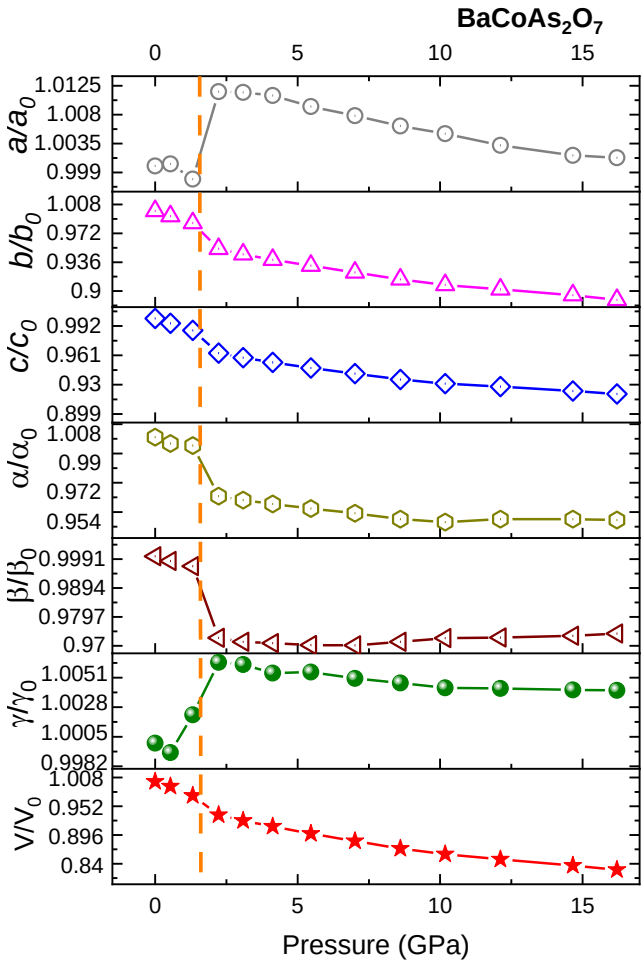

Figure S1 Pressure dependent cell parameters and volume for $BaCoAs_2O_7$ obtained from Lebail refinement of the preliminary laboratory X-ray diffraction experiments.

Table S1 Pressure dependent cell parameters and volume for $BaCoAs_2O_7$ obtained from Lebail refinement of preliminary laboratory x-ray experiments.

P(GPa)	a(Å)	b(Å)	c(Å)	α(°)	β(°)	γ(°)	Vol(Å^3)	R_p	R_{wp}	χ2
0	5.5447(4)	7.7699(5)	7.2983(5)	101.55(1)	83.50(1)	88.36(1)	305.34(6)	10.5	8.74	0.054
0.54	5.5464(4)	7.7195(6)	7.2613(6)	101.16(1)	83.37(2)	88.30(1)	302.54(9)	7.82	6.04	0.026
1.33	5.5333(4)	7.6526(6)	7.2058(5)	101.04(1)	83.22(1)	88.56(1)	297.03(4)	12.1	9.37	0.089
2.23	5.6089(6)	7.4022(7)	7.0312(6)	97.87(1)	81.21(1)	88.92(1)	285.55(4)	11.5	10.2	0.210
3.09	5.6082(6)	7.3484(7)	6.9960(6)	97.62(1)	81.10(1)	88.91(1)	282.10(4)	13.2	11.5	0.245
4.12	5.6056(6)	7.2962(7)	6.9597(7)	97.38(1)	81.07(1)	88.85(1)	278.64(5)	14.8	12.8	0.27
5.47	5.5960(6)	7.2386(6)	6.9165(6)	97.10(1)	81.01(1)	88.85(1)	274.39(4)	13.9	11.8	0.325
7.01	5.5881(6)	7.1733(6)	6.8726(7)	96.80(1)	81.01(1)	88.82(1)	269.97(5)	12.7	10.4	0.196
8.60	5.5792(6)	7.1060(7)	6.8273(9)	96.43(1)	81.10(1)	88.78(1)	265.53(5)	13.9	11.2	0.226
10.18	5.5726(6)	7.0521(6)	6.7962(8)	96.25(2)	81.21(1)	88.75(1)	262.17(5)	15.6	12.5	0.363

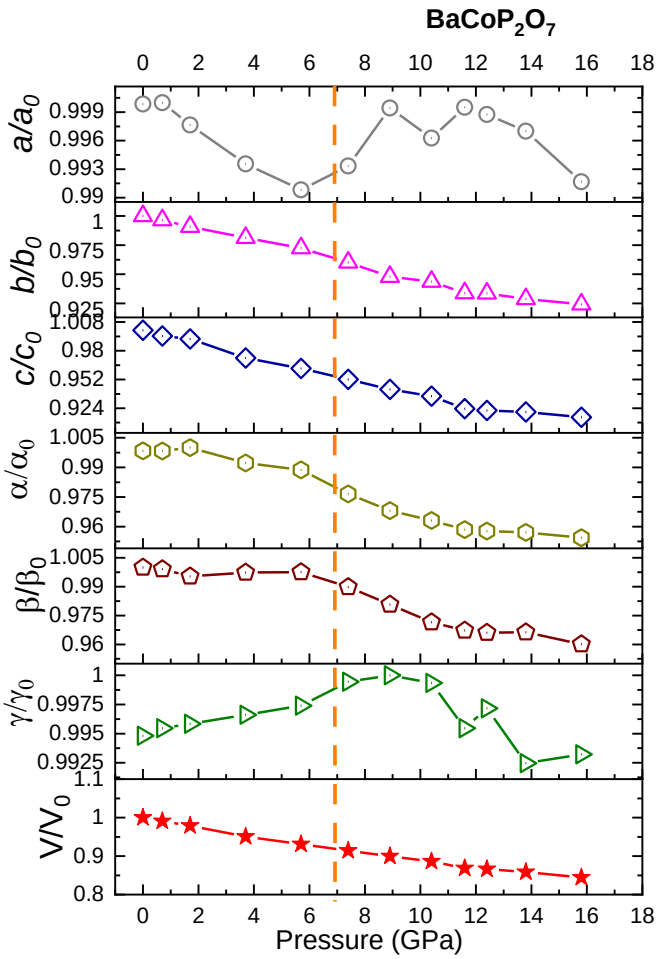

Figure S2 Pressure dependent cell parameters and volume for $BaCoP_2O_7$ obtained from Lebail refinement of preliminary laboratory X-ray diffraction experiments.

Table S2 Pressure dependent cell parameters and volume for $BaCoP_2O_7$ obtained from Lebail refinement of preliminary laboratory x-ray experiments.

P(GPa)	a(Å)	b(Å)	c(Å)	α(°)	β(°)	γ(°)	Vol(Å^3)	R_p	R_{wp}	$\chi 2$
0	5.3566(13)	7.5818(19)	7.1646(21)	102.01(1)	85.25(1)	88.95(1)	283.44(13)	6.97	6.10	0.067
0.7	5.3574 (8)	7.5549(11)	7.1244(15)	102.00(1)	85.17(2)	89.01(1)	280.88(8)	7.71	6.81	0.025
1.7	5.3448(8)	7.5120(10)	7.5120(11)	102.18(1)	84.85(1)	89.04(1)	277.50(7)	12.3	11.0	0.083
3.7	5.3228(6)	7.4401(9)	6.9711(10)	101.38(1)	85.01(1)	89.11(1)	269.47(6)	7.91	6.93	0.034
5.7	5.3082(7)	7.3727(11)	6.8978(12)	101.02(1)	85.04(1)	89.18(1)	263.85(7)	8.96	8.43	0.039
7.4	5.3229(8)	7.2788(11)	6.8204(11)	99.75(1)	84.37(1)	89.35(1)	259.07(7)	14.9	14.9	0.137
8.9	5.3543(9)	7.1870(13)	6.7513(12)	98.92(1)	83.60(1)	89.41(1)	254.96(7)	17.3	15.3	0.138
10.4	5.3374(10)	7.1548(12)	6.7042(10)	98.40(1)	82.81(1)	89.35(1)	251.17(1)	14.7	14.0	0.12
11.6	5.3548(10)	7.0802(8)	6.6165(15)	97.93(1)	82.46(1)	89.01(1)	246.14(7)	16	17	0.196
12.4	5.3508(10)	7.0787(9)	6.6050(15)	97.86(1)	82.35(1)	89.16(1)	245.49(8)	18.5	18.9	0.211
13.8	5.3413(10)	7.0416(8)	6.5938(15)	97.79(1)	82.38(1)	88.74(1)	243.34(7)	17.7	18.5	0.193
15.8	5.31287(9)	7.0071(9)	6.5570(17)	97.51(1)	81.85(1)	88.81(1)	239.37(8)	20.8	21	0.23

Table S3 Pressure dependence unit cell parameters and the unit volumes from the synchrotron x-ray powder diffraction (SXRPD) refinement of $BaCoAs_2O_7$ compounds with the coexistence of low-pressure phase and high-pressure phase refined parameters around the phase transitions on compression.

P(GPa)	a(Å)	b(Å)	c(Å)	α(°)	β(°)	γ(°)	Vol(Å^3)	R_p	R_{wp}	χ2
0.55(1)	5.5397(1)	7.7370(5)	7.2708(4)	101.41(1)	83.46(1)	88.42(1)	303.09(3)	16	15.6	0.981
0.80(1)	5.5384(1)	7.7256(5)	7.2581(4)	101.39(1)	83.42(1)	88.45(1)	302.04(3)	15.3	14.1	0.832
0.95(1)	5.5373(1)	7.7177(5)	7.2490(4)	101.31(1)	83.38(1)	88.45(1)	301.35(3)	18.1	15.4	0.929
1.05(1)	5.5364(2)	7.7108(5)	7.2418(4)	101.25(1)	83.35(1)	88.45(1)	300.79(3)	19.7	17.6	1.13
1.20(1)	5.5356(2)	7.7013(5)	7.2339(4)	101.18(1)	83.32(1)	88.45(1)	300.09(3)	15.9	14.3	0.825
1.30(1)	5.5346(2)	7.6936(5)	7.2265(4)	101.11(1)	83.30(1)	88.45(1)	299.49(3)	16	14.2	0.784
1.35(1)	5.5342(2)	7.6858(5)	7.2183(4)	101.06(1)	83.27(1)	88.47(1)	298.87(3)	26.6	15.8	0.928
1.45(1)	5.5345(2)	7.6796(5)	7.2127(4)	101.03(1)	83.26(1)	88.48(1)	298.44(3)	19.2	16.3	0.917
1.50(1)	5.5345(2)	7.6749(5)	7.2080(4)	100.99(1)	83.24(1)	88.48(1)	298.08(3)	17.6	14.4	0.736
1.55(1)	5.5347(2)	7.6655(5)	7.2006(4)	100.92(1)	83.18(1)	88.49(1)	297.46(3)	14.4	12.1	0.569
1.65(1)	5.5342(3)	7.6567(5)	7.1912(4)	100.85(1)	83.15(1)	88.50(1)	296.76(3)	14.5	11.3	0.458
1.80(1)	5.5351(0)	7.6386(0)	7.1752(0)	100.70(0)	83.08(1)	88.51(1)	295.56(0)	12.4	9.73	0.316
1.95(1)	5.5296(4)	7.6306(5)	7.1696(4)	100.68(0)	83.09(1)	88.51(1)	294.75(4)	11.3	9.3	0.285
2.15(1)	5.5209(9)	7.6227(8)	7.1520(6)	100.65(0)	83.12(1)	88.50(1)	293.31(6)	13.5	10.3	0.335
2.25(1)	5.5335(9)	7.6049(9)	7.1493(9)	100.67(2)	83.31(1)	88.48(1)	293.28(5)	12	9.3	0.303
2.45(1)	5.5893(5)	7.4562(6)	7.0349(5)	98.27(1)	82.04(1)	89.20(1)	287.16(4)	15.8	12.1	0.399
2.70(1)	5.5886(5)	7.4342(6)	7.0261(5)	98.14(1)	81.71(1)	89.10(1)	285.75(4)	12.6	9.7	0.438
3.00(1)	5.5892(6)	7.4070(6)	7.0223(4)	98.10(1)	81.45(1)	88.95(1)	284.39(4)	10.8	8.38	0.32
3.35(1)	5.5908(4)	7.3925(4)	6.9972(8)	97.74(1)	81.40(1)	89.01(1)	283.13(4)	11	8.4	0.317
3.60(1)	5.5903(5)	7.3707(5)	6.9924(7)	97.83(1)	81.22(1)	88.94(1)	281.86(4)	11.4	8.52	0.258
3.95(1)	5.5869(5)	7.3596(5)	6.9804(6)	97.83(1)	81.18(1)	88.99(1)	280.76(4)	11.7	8.76	0.274
4.40(1)	5.5839(5)	7.3398(5)	6.9699(6)	97.77(1)	81.12(1)	88.99(1)	279.43(4)	10.7	8.19	0.253
5.10(1)	5.5747(9)	7.2969(7)	6.9240(7)	96.81(2)	81.48(1)	88.87(1)	276.39(6)	14.6	11.0	0.417
1.80(1)	5.5935(0)	7.4322(0)	7.0300(0)	98.24(0)	82.03(0)	89.20(0)	286.27(0)	12.4	9.73	0.316
1.95(1)	5.5935(0)	7.4322(0)	7.0300(0)	98.24(0)	82.03(0)	89.20(0)	286.27(0)	11.3	9.3	0.285
2.15(1)	5.5875 (7)	7.4234(17)	7.0415(17)	98.25(0)	82.03(0)	89.20(0)	286.09(9)	13.5	10.3	0.335
2.25(1)	5.5872(5)	7.4497(12)	7.0372(5)	98.18(1)	82.17(1)	89.26(0)	287.07(9)	12	9.3	0.303

Table S4 Pressure dependence unit cell parameters and the unit volumes from the SXRPD refinement of $BaCoP_2O_7$ compounds with the coexistence of low-pressure and high-pressure phase refined parameters around the phase transitions on compression.

P(GPa)	a(Å)	b(Å)	c(Å)	α(°)	β(°)	γ(°)	Vol(Å^3)	R_p	R_{wp}	χ2
4.2(1)	5.3265(3)	7.4193(9)	6.9568(6)	101.19(1)	85.26(1)	88.95(1)	268.61(4)	15.7	32.1	6.52
4.4(1)	5.3258(3)	7.4150(9)	6.9523(6)	101.23(1)	85.23(1)	88.96(1)	268.20(4)	14.9	31	6.24
4.5(1)	5.3229(5)	7.4155(15)	6.9401(9)	101.05(1)	85.33(1)	88.97(1)	267.80(7)	16.8	46	14.2
4.8(1)	5.3178(4)	7.3996(10)	6.9354(7)	101.11(1)	85.28(1)	89.00(1)	266.74(4)	26.4	43.5	11.9
5.6(1)	5.3155(2)	7.3739(7)	6.9084(5)	101.05(1)	85.20(1)	89.01(1)	264.67(4)	11.9	23.3	3.17
6(1)	5.3128(2)	7.3438(7)	6.8891(5)	100.92(1)	85.00(1)	89.02(1)	262.76(4)	16.7	25.8	3.21
6.3(1)	5.3092(3)	7.3322(8)	6.8749(6)	100.71(1)	84.99(1)	89.07(1)	261.82(4)	17.6	27.4	3.54
6.6(1)	5.3100(3)	7.3176(8)	6.8594(7)	100.52(1)	84.93(1)	89.07(1)	260.88(4)	19.2	30.5	4.49
6.8(1)	5.3100(0)	7.3176(0)	6.8594(0)	100.52(0)	84.93(0)	89.07(0)	260.88(0)	14.1	24.5	2.68
6.95(1)	5.3063(4)	7.3066(0)	6.8574(0)	100.50(0)	84.93(0)	89.07(0)	260.25(4)	16.4	28.2	3.19
7.05(1)	5.3166(2)	7.2935(10)	6.8318(0)	100.20(0)	84.71(0)	89.15(0)	259.48(7)	15.5	27.2	3.18
7.2(1)	5.31386(7)	7.2946(11)	6.8218(12)	100.09(1)	84.79(2)	89.07(1)	259.13(7)	14.8	31.0	4.17
7.3(1)	5.3511(5)	7.2156(8)	6.7884(10)	98.84(1)	83.98(1)	89.14(1)	257.44(5)	19.6	35.0	6.14
7.45(1)	5.3520(4)	7.2025(8)	6.7871(9)	98.80(1)	83.87(1)	89.17(1)	256.94(5)	18.7	31.7	5.14
7.7(1)	5.3501(3)	7.1913(9)	6.7814(10)	98.61(1)	83.75(1)	89.16(1)	256.30(5)	19.2	33.1	4.27
7.8(1)	5.3502(3)	7.1797(9)	6.7691(10)	98.45(1)	83.65(1)	89.18(1)	255.50(5)	20.3	32.4	4.07
8(1)	5.3531(3)	7.1638(7)	6.7582(12)	98.01(1)	83.68(1)	88.97(1)	254.94(5)	21.9	35.5	4.90
8.2(1)	5.3540(3)	7.1544(8)	6.7379(10)	98.09(1)	83.50(1)	89.06(1)	253.75(5)	18.2	29.4	3.64
8.4(1)	5.3532(3)	7.1486(8)	6.7378(10)	98.26(1)	83.46(1)	89.04(1)	253.36(5)	17.6	33.7	6.01
8.6(1)	5.3535(3)	7.1383(8)	6.7276(10)	98.16(1)	83.40(1)	89.01(1)	252.65(5)	17.3	32.6	5.67
8.75(1)	5.3524(4)	7.1333(9)	6.7245(9)	98.20(1)	83.35(1)	89.01(1)	252.26(5)	19.5	38	8.22
9.35(1)	5.3503(4)	7.1120(8)	6.7061(9)	98.00(1)	83.22(1)	88.98(1)	250.78(5)	19.2	36.6	7.63
9.6(1)	5.3482(4)	7.1026(7)	6.7032(8)	97.89(1)	83.18(1)	88.96(1)	250.28(5)	19	34.4	6.73
9.75(1)	5.3432(3)	7.0884(6)	6.7148(8)	97.55(1)	83.18(1)	88.96(1)	250.19(4)	16.7	29.6	4.14
10(1)	5.3481(3)	7.0784(7)	6.6916(8)	97.44(1)	83.06(1)	88.90(1)	249.19(4)	20.1	31.7	4.76
10.2(1)	5.3459(3)	7.0683(7)	6.6862(8)	97.39(1)	83.04(1)	88.88(1)	248.55(4)	19.6	32.7	5.17
10.4(1)	5.3431(3)	7.0593(7)	6.6832(8)	97.335(1)	83.03(1)	88.85(1)	248.02(4)	18.1	30.8	4.69
10.9(1)	5.3414(3)	7.0503(8)	6.6761(8)	97.246(1)	83.04(1)	88.81(1)	247.40(5)	17.8	33.1	5.46

11.05(1)	5.3383(3)	7.0337(6)	6.6684(7)	97.08(1)	83.01(1)	88.75(1)	246.46(4)	16.8	28.3	4.15
11.45(1)	5.3371(4)	7.0253(9)	6.6618(8)	96.98(1)	83.00(1)	88.69(1)	245.90(5)	17.6	32.3	5.54
11.65(1)	5.3383(5)	7.0187(10)	6.6514(7)	96.92(1)	82.97(1)	88.60(1)	245.35(5)	17.4	32	5.34
11.95(1)	5.3394(3)	7.0015(6)	6.6461(8)	96.82(1)	82.84(1)	88.69(1)	244.59(4)	14.6	25.5	3.39
12.25(1)	5.3375(3)	6.9930(6)	6.6417(9)	96.75(1)	82.78(1)	88.69(1)	244.06(4)	14.4	25	3.38
12.6 (1)	5.3354(3)	6.9826(6)	6.6387(9)	96.68(1)	82.73(1)	88.69(1)	243.50(4)	13.9	23.3	3.01
12.95(1)	5.3341(3)	6.9721(6)	6.6298(10)	96.59(1)	82.68(1)	88.66(1)	242.76(4)	14.4	24.8	3.44
13.4(1)	5.3329(3)	6.9560(6)	6.6167(10)	96.47(1)	82.61(1)	88.62(1)	241.68(5)	14.1	23.6	3.10
13.85(1)	5.3312(3)	6.9407(7)	6.6071(11)	96.36(1)	82.55(1)	88.62(1)	240.74(5)	14.8	24.2	3.26
14.45(1)	5.3296(4)	6.9254(7)	6.5937(12)	96.27(1)	82.52(1)	88.57(1)	239.67(5)	14.4	25.4	3.49
15.05(1)	5.3263(4)	6.9146(8)	6.5859(12)	96.22(1)	82.45(1)	88.59(1)	238.85(5)	15.1	25.5	3.48
15.55(1)	5.3233(3)	6.8957(9)	6.5703(12)	96.12(1)	82.39(1)	88.56(1)	237.52(5)	15.3	24.8	3.20
16.25(1)	5.3180(4)	6.8809(10)	6.5624(11)	96.07(1)	82.32(1)	88.54(1)	236.45(6)	16.3	25.1	3.36
16.95(1)	5.3152(4)	6.8612(11)	6.5392(11)	95.90(1)	82.29(1)	88.40(1)	234.86(6)	16.3	25.5	3.55
17.5(1)	5.3114(4)	6.8525(11)	6.5233(10)	95.78(1)	82.24(1)	88.32(1)	233.83(6)	16.4	25.6	3.63
18.05(1)	5.3076(4)	6.8430(9)	6.5172(11)	95.79(1)	82.19(1)	88.20(1)	233.07(6)	15.5	24.4	3.34
18.65(1)	5.3052(4)	6.8374(10)	6.5035(11)	95.79(1)	82.19(1)	88.27(1)	232.30(6)	14.7	23.7	3.07

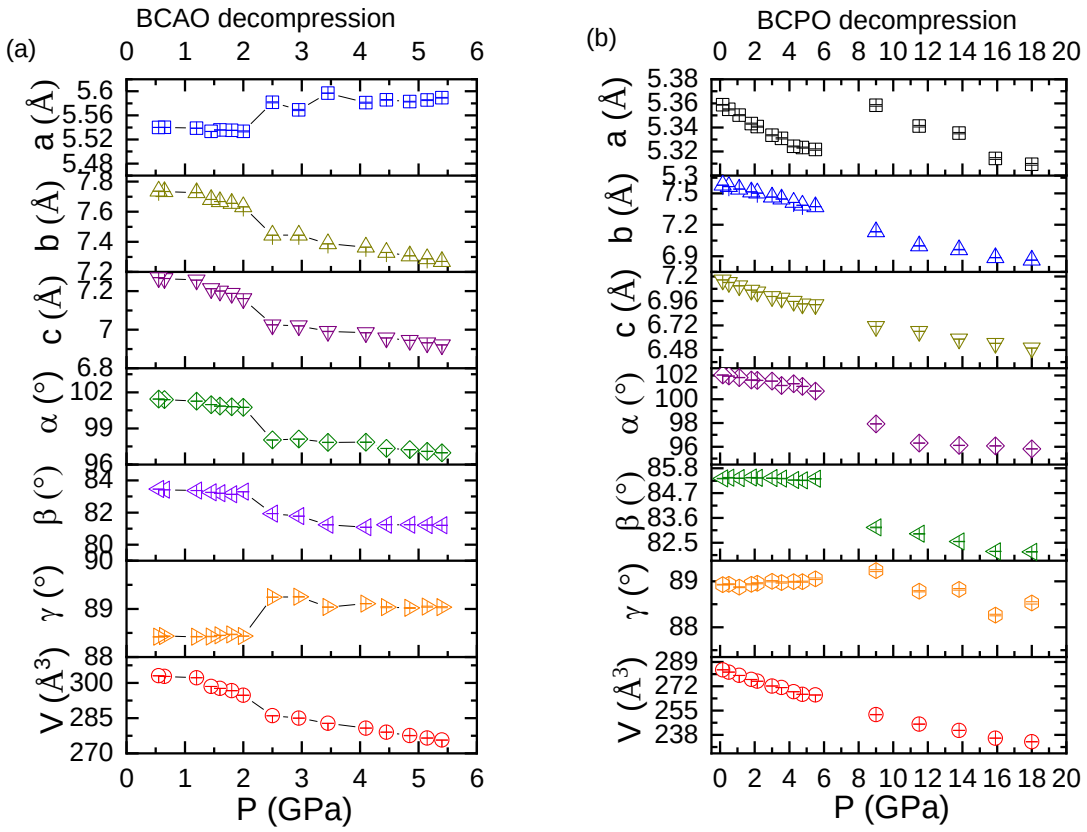

Figure S3 Pressure evolution lattice cell parameters and volume on decompression of (a) BCAO from 5.4 GPa to 0.55 GPa and (b) BCPO from 18 GPa to 0.15 GPa obtained from synchrotron x-ray powder diffraction refinements.

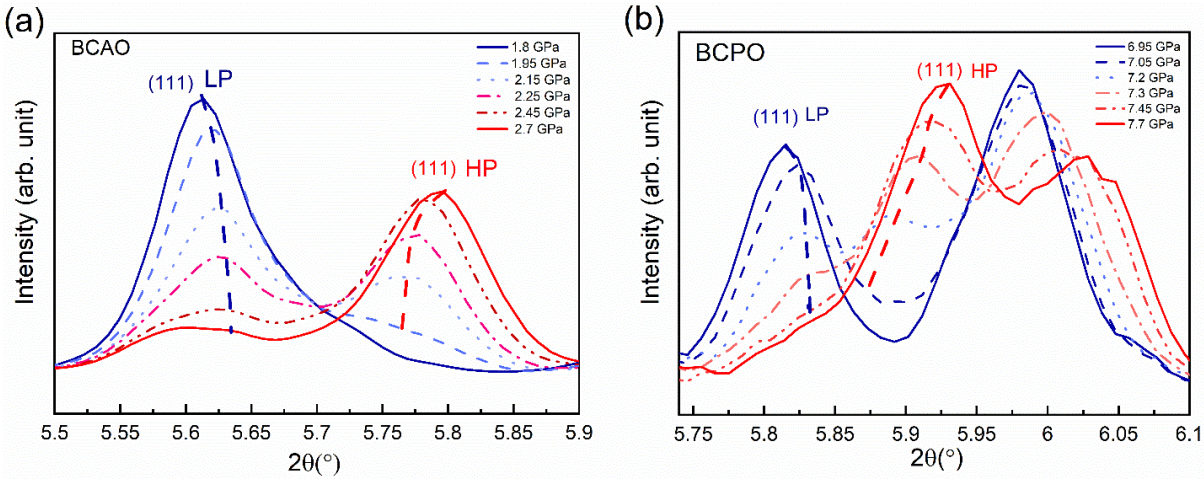

Figure S4 The zoomed portion of pressure evolution synchrotron diffraction pattern around the phase transition regions shows the coexistence of low pressure and high-pressure phase around the phase transition regions of (a) BCAO and (b) BCPO. The dashed lines are guide for the eye to indicate the Bragg peak positions.

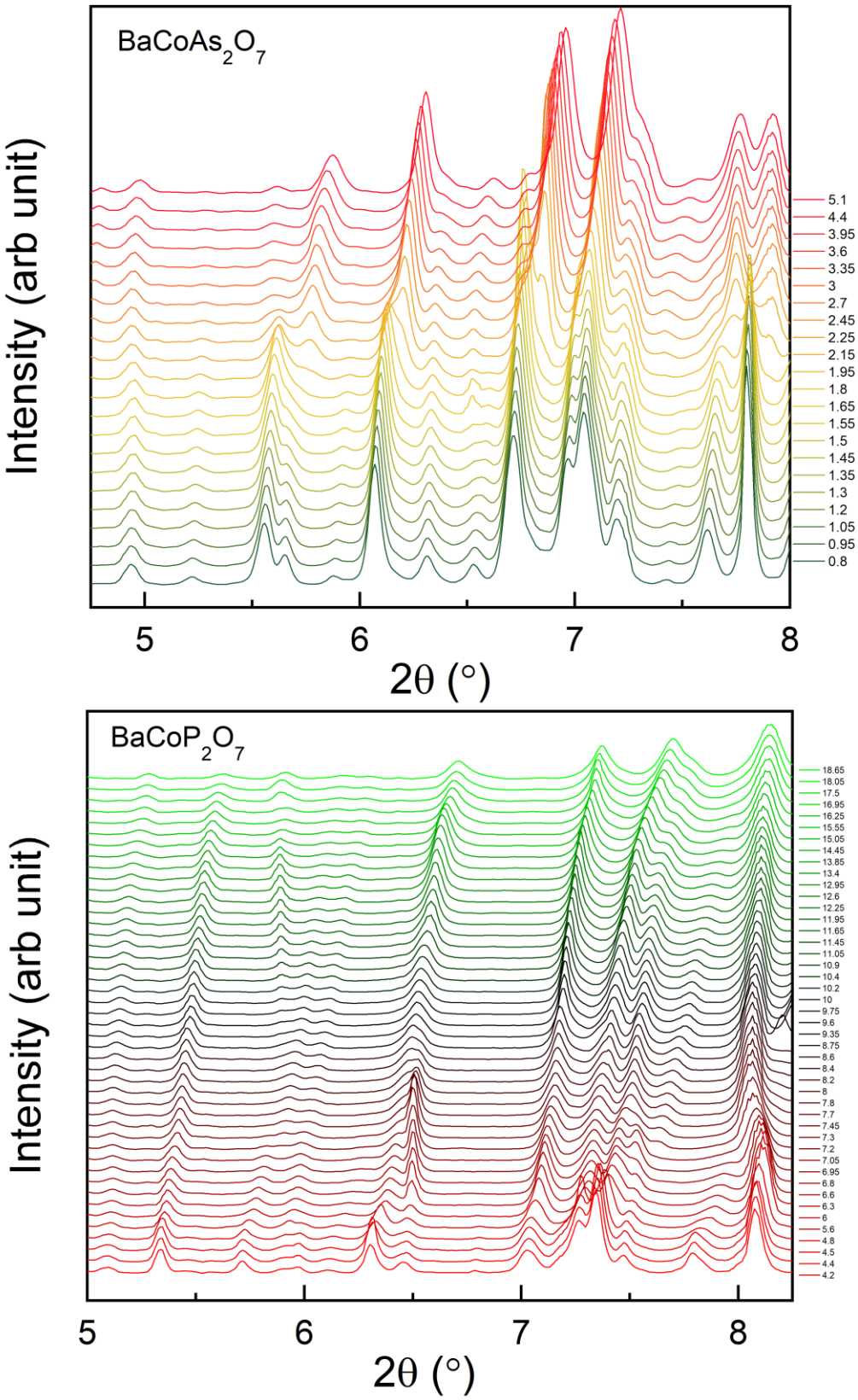

Figure S5 Diffraction pattern obtained at different pressure presented for $BaCoAs_2O_7$ (upper panel) and $BaCoP_2O_7$ (lower panel) as a supplementary figure to the Figure 3. Pressure units are in GPa.

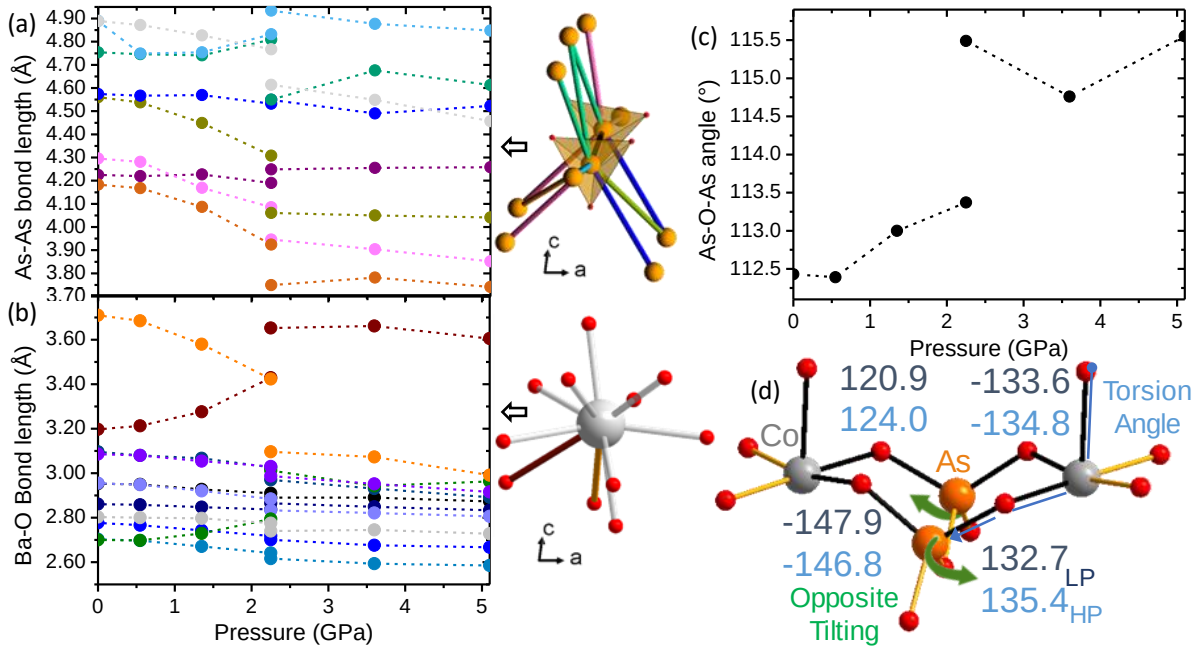

Figure S6 Additional plots for evolution of selected bond lengths (Å) vs Pressure (GPa) values extracted from DFT- relaxed synchrotron XRD experiments structural models (Lattice parameters for DFT were constrained to the refined values): (a) in the case of As-As bonds (b) In the case of Ba-O bonds and (c) in the case of As-O-As bridge angle (°). (d) Comparison of O-Co-O-As tilting angles (°) between 1.35 GPa low-pressure values (dark-blue) and 3.6 GPa high-pressure value (light-blue).